

=> fil casrea; d stat que 146
 FILE 'CASREACT' ENTERED AT 16:51:26 ON 12 MAR 2007
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FILE CONTENT:1840 - 11 Mar 2007 VOL 146 ISS 11

New CAS Information Use Policies, enter HELP USAGETERMS for details.

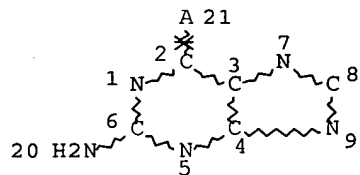
```
*****
*
*      CASREACT now has more than 12 million reactions      *
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database, compiled under the direction of Professor Dr. Klaus Kieslich.

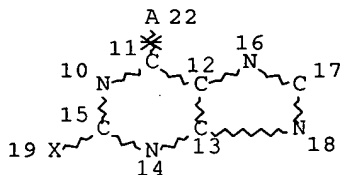
This file contains CAS Registry Numbers for easy and accurate substance identification.

L1 STR

RRT



PRO



NODE ATTRIBUTES:

NSPEC IS RC AT 21
 NSPEC IS RC AT 22
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

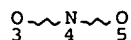
RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

****MAPPINGS****

NOD SYM	ROL	NOD SYM	ROL
21 A	RRT	22 A	PRO
22 A	PRO	21 A	RRT

L4 81 SEA FILE=CASREACT SSS FUL L1 (264 REACTIONS)
 L20 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

L23 76 SEA FILE=CASREACT SUB=L4 SSS FUL L20 (250 REACTIONS)

L25 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 2

STEREO ATTRIBUTES: NONE

L28 8 SEA FILE=CASREACT SUB=L4 SSS FUL L25 (18 REACTIONS)

L29 7 SEA FILE=CASREACT ABB=ON L28 AND L23

L46 7 SEA FILE=CASREACT ABB=ON L29 OR (L29 AND (L23 OR L28))

=> fil capl; d stat que l44

FILE 'CAPLUS' ENTERED AT 16:51:31 ON 12 MAR 2007

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FILE COVERS 1907 - 12 Mar 2007 VOL 146 ISS 12

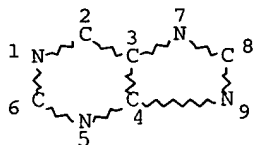
FILE LAST UPDATED: 11 Mar 2007 (20070311/ED)

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<http://www.cas.org/infopolicy.html>

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

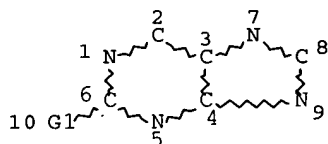
L5 184754 SEA FILE=REGISTRY ABB=ON X/ELS AND SI/ELS
L30 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L31 258797 SEA FILE=REGISTRY SSS FUL L30
L32 STR



VAR G1=NH2/X
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L35 62619 SEA FILE=REGISTRY SUB=L31 SSS FUL L32
L36 13779 SEA FILE=REGISTRY ABB=ON L35 AND X/ELS
L37 48840 SEA FILE=REGISTRY ABB=ON L35 NOT L36
L38 93825 SEA FILE=CAPLUS ABB=ON L37
L39 3461 SEA FILE=CAPLUS ABB=ON L36/P
L40 9922 SEA FILE=CAPLUS ABB=ON L38(L) RACT/RL
L41 177552 SEA FILE=CAPLUS ABB=ON L5
L42 207 SEA FILE=CAPLUS ABB=ON L39 AND L40 AND L41
L43 56042 SEA FILE=CAPLUS ABB=ON NITRITE#/OBI
L44 4 SEA FILE=CAPLUS ABB=ON L43 AND L42

=> dup rem 146,144
FILE 'CASREACT' ENTERED AT 16:51:39 ON 12 MAR 2007
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PROCESSING COMPLETED FOR L46

PROCESSING COMPLETED FOR L44

L47 11 DUP REM L46 L44 (0 DUPLICATES REMOVED)

ANSWERS '1-7' FROM FILE CASREACT

ANSWERS '8-11' FROM FILE CAPLUS

=> d ibib abs hit

L47 ANSWER 1 OF 11 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 145:62710 CASREACT Full-text

TITLE: Structure and Synthesis of 6-(Substituted-imidazol-1-yl)purines: Versatile Substrates for Regiospecific Alkylation and Glycosylation at N9

AUTHOR(S): Zhong, Minghong; Nowak, Ireneusz; Cannon, John F.; Robins, Morris J.

CORPORATE SOURCE: Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, 84602-5700, USA

SOURCE: Journal of Organic Chemistry (2006), 71(11), 4216-4221
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

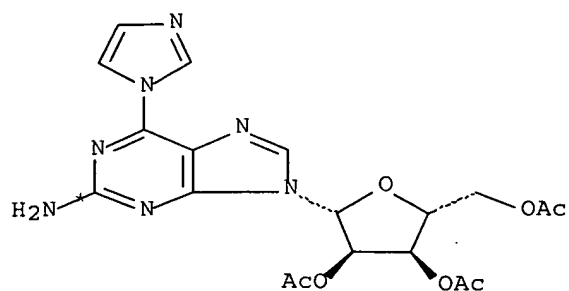
DOCUMENT TYPE: Journal

LANGUAGE: English

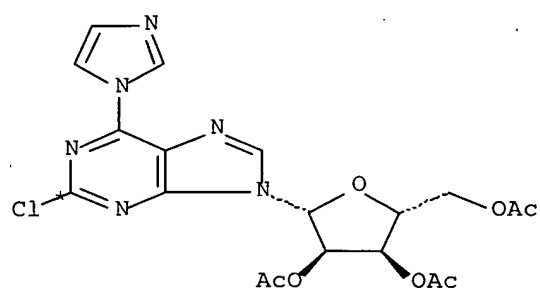
AB X-ray crystal structures of several 6-(azolyl)purine base and nucleoside derivs. show essentially coplanar conformations of the purine and appended 6-(azolyl) rings. However, the planes of the purine and imidazole rings are twisted .apprx.57° in a 2-chloro-6-(4,5-diphenyl-imidazol-1-yl)purine nucleoside, and a twist angle of .apprx.61° was measured between the planes of the purine and pyrrole rings in the structure of a 6-(2,5-dimethyl-pyrrol-1-yl)purine nucleoside derivative. Shielding "above" N7 of the purine ring by a proximal C-H on the 6-azolyl moiety is apparent with the coplanar compds., but this effect is diminished in those without coplanarity. Syntheses of 6-(azolyl)purines from both base and nucleoside starting materials are described. Treatment of 2,6-dichloropurine with imidazole gave 2-chloro-6-(imidazol-1-yl)purine. Modified Appel reactions at C6 of trityl-protected hypoxanthine and guanine derivs. followed by detritylation gave 6-(imidazol-1-yl)- and 2-amino-6-(imidazol-1-yl)purines. Imidazole was introduced at C6 of 2',3',5'-tri-O-acetyl- inosine by a modified Appel reaction, and solvolysis of the glycosyl linkage gave 6-(imidazol-1-yl)purine. Guanosine triacetate was transformed into the protected 2,6-dichloropurine nucleoside, which was subjected to SNAr displacement with imidazoles at C6 followed by glycosyl solvolysis to provide 2-chloro-6-(substituted-imidazol-1-yl)purines. Potential applications of these purine derivs. are outlined.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(10) OF 40 ...AE ==> AC...



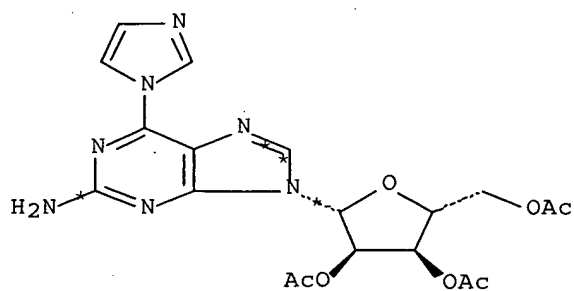
AE

(10)
→AC
YIELD 81%

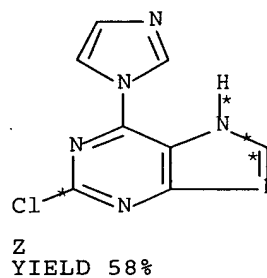
RX(10) RCT AE 891497-84-0
 RGT AF 121699-36-3 Benzenemethanaminium, N,N,N-triethyl-,
 nitrite, AG 75-77-4 Me3SiCl
 PRO AC 891497-83-9
 SOL 75-09-2 CH2Cl2
 CON overnight, room temperature

RX(27) OF 40 COMPOSED OF RX(10), RX(8)

RX(27) AE ==> Z



AE

2
STEPS
→Z
YIELD 58%

RX(10) RCT AE 891497-84-0

RGT AF 121699-36-3 Benzenemethanaminium, N,N,N-triethyl-,
 nitrite, AG 75-77-4 Me3SiCl
 PRO AC 891497-83-9
 SOL 75-09-2 CH2Cl2
 CON overnight, room temperature

RX(8) RCT AC 891497-83-9

STAGE(1)

RGT T 75-36-5 AcCl
 SOL 64-19-7 AcOH
 CON 11 hours, 65 deg C

STAGE(2)

RGT P 1310-73-2 NaOH
 SOL 7732-18-5 Water
 CON room temperature

STAGE(3)

RGT Q 124-38-9 CO2
 CON room temperature, neutralized

PRO Z 891497-82-8

=> d ibib abs hit 2-7; d ibib ed abs hitstr 8-11; fil hom

L47 ANSWER 2 OF 11 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:347381 CASREACT Full-text

TITLE: Synthesis and Reactions of 2-Chloro- and
 2-Tosyloxy-2'-deoxyinosine Derivatives

AUTHOR(S): Pottabathini, Narender; Bae, Suyeal; Pradhan,
 Padmanava; Hahn, Hoh-Gyu; Mah, Heduck; Lakshman,
 Mahesh K.

CORPORATE SOURCE: Department of Chemistry, The City College and The City
 University of New York, New York, NY, 10031-9198, USA

SOURCE: Journal of Organic Chemistry (2005), 70(18), 7188-7195
 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

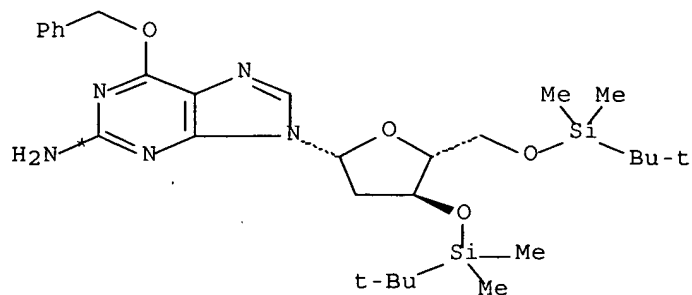
LANGUAGE: English

AB Convenient syntheses of 2-chloro- and 2-tosyloxy-2'-deoxyinosine as their
 tert-butyldimethylsilyl ethers are described. Both compds. can be synthesized
 via a common route and rely on com. available 2'-deoxyguanosine. The present
 method leading to the chloro nucleoside is operationally simpler compared to
 previously reported glycosylation techniques where isomeric products were
 obtained. Both electrophilic nucleosides can be used for the preparation of
 N-substituted 2'-deoxyguanosine analogs via displacement of the leaving
 groups, and a comparison of their reactivities shows the chloro analog to be
 superior. Interestingly, a Pd catalyst-mediated, two-step, one-pot conversion
 of an allyl-protected chloro nucleoside intermediate to the final modified 2'-
 deoxyguanosine derivs. is also feasible. On the basis of these observations,
 initial assessments of Pd-catalyzed aryl amination as well as a C-C cross-
 coupling have also been performed with the chloro and tosyloxy nucleoside
 substrates. Results indicate a potentially high synthetic utility of 2-
 chloro-2'-deoxyinosine and in many instances this derivative can supplant the
 bromo and fluoro analogs that are more cumbersome to prepare or are not
 readily available.

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS

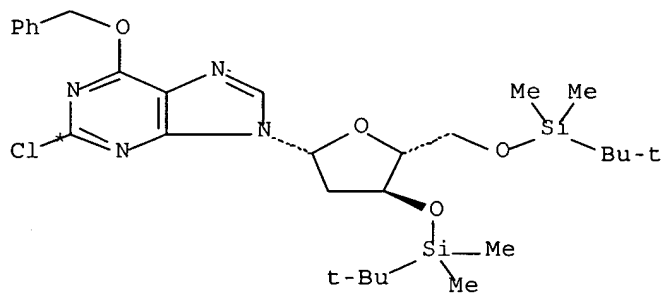
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 62 A ==> B...



A

(1) →



B

RX(1)

STAGE(1)

RGT C 540-80-7 t-BuONO

SOL 75-09-2 CH₂Cl₂

CON room temperature -> -10 deg C

STAGE(2)

RCT A 236427-57-9

RGT D 75-77-4 Me₃SiClSOL 75-09-2 CH₂Cl₂

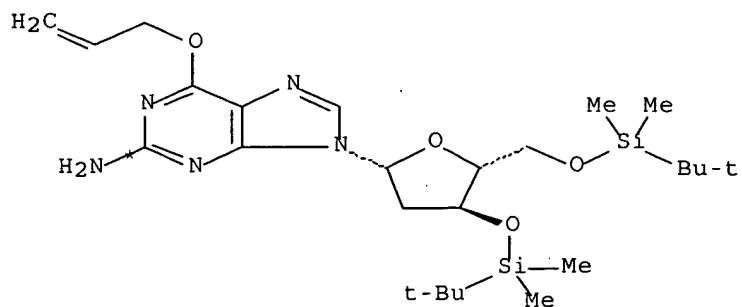
CON 2 hours, -10 deg C

STAGE(3)

RGT E 144-55-8 NaHCO₃SOL 7732-18-5 Water, 75-09-2 CH₂Cl₂

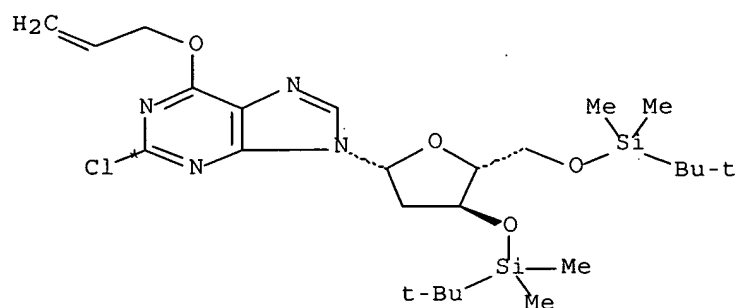
PRO B 865710-39-0

RX(2) OF 62 H ==> I...



H

(2) →



I

YIELD 52%

RX(2)

STAGE(1)

RGT C 540-80-7 t-BuONO

SOL 75-09-2 CH₂Cl₂

CON room temperature -> -10 deg C

STAGE(2)

RGT H 150903-99-4

RGT D 75-77-4 Me₃SiClSOL 75-09-2 CH₂Cl₂

CON 2 hours, -10 deg C

STAGE(3)

RGT E 144-55-8 NaHCO₃SOL 7732-18-5 Water, 75-09-2 CH₂Cl₂

PRO I 865710-40-3

L47 ANSWER 3 OF 11 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 142:392592 CASREACT Full-text

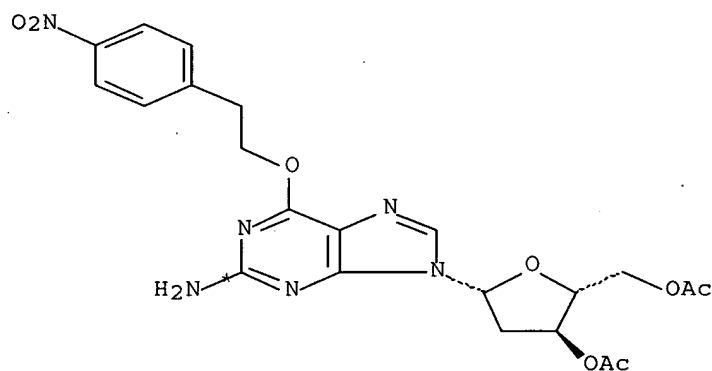
TITLE: Synthesis of Adducts of o-Quinone Metabolites of
 Carcinogenic Polycyclic Aromatic Hydrocarbons with
 2'-Deoxyribonucleosides

AUTHOR(S): Dai, Qing; Ran, Chongzhao; Harvey, Ronald G.
 CORPORATE SOURCE: Ben May Institute for Cancer Research, The University
 of Chicago, Chicago, IL, 60637, USA
 SOURCE: Organic Letters (2005), 7(6), 999-1002
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The first syntheses of the adducts formed in the reactions of o-quinone
 metabolites of carcinogenic polycyclic aromatic hydrocarbons (BPQ and BAQ) at
 2'-deoxyadenosine and 2'-deoxyguanosine sites in DNA are reported. These
 syntheses entail Pd-catalyzed coupling of protected amine derivs. of catechols
 with suitably protected halopurine analogs of 2'-deoxyribonucleosides.

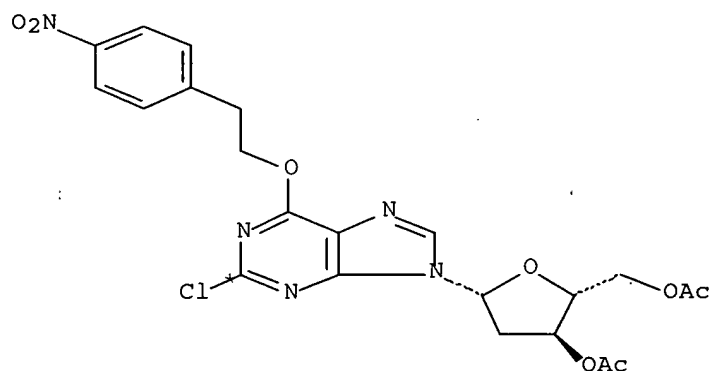
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(4) OF 143 P ==> Q...



P

(4) →



Q
 YIELD 75%

RX(4) RCT P 108310-92-5

STAGE(1)

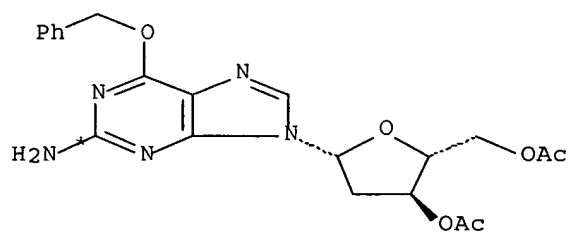
RGT K 540-80-7 t-BuONO, L 75-77-4 Me3SiCl
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 1 hour, 0 deg C

STAGE(2)

RGT M 144-55-8 NaHCO3
 SOL 7732-18-5 Water
 CON 0 deg C

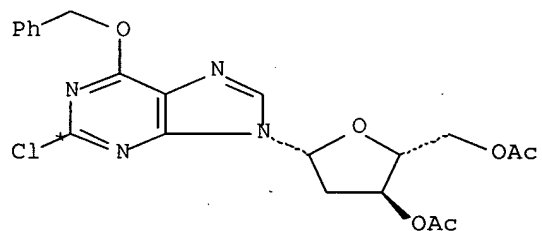
PRO Q 849830-82-6

RX(5) OF 143 R ==> S...



R

(5)
 →



S
 YIELD 60%

RX(5) RCT R 144640-75-5

STAGE(1)

RGT K 540-80-7 t-BuONO, L 75-77-4 Me3SiCl
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 1 hour, 0 deg C

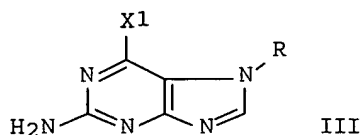
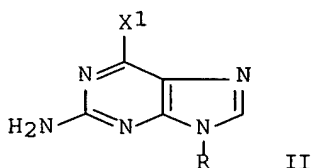
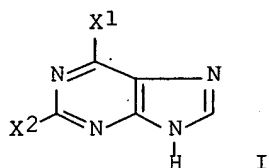
STAGE(2)

RGT M 144-55-8 NaHCO3
 SOL 7732-18-5 Water
 CON 0 deg C

PRO S 849830-81-5

L47 ANSWER 4 OF 11 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 139:307792 CASREACT Full-text
 TITLE: Regioselective halogenation method for the production
 of 2,6-dihalopurines
 INVENTOR(S): Hayashi, Taketo; Kumazawa, Hiroharu; Kawakami,
 Takehiko
 PATENT ASSIGNEE(S): Sumika Fine Chemicals Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 19 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

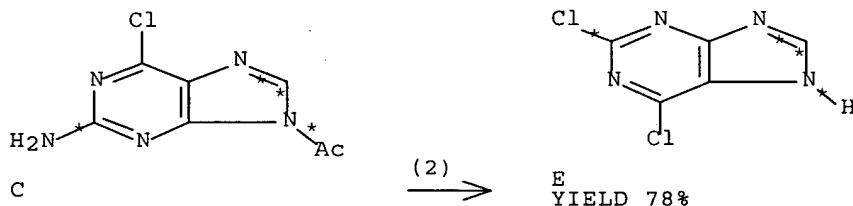
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003084958	A1	20031016	WO 2003-JP4259	20030403
W:			AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW	
RW:			GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG	
AU 2003226448	A1	20031020	AU 2003-226448	20030403
EP 1490369	A1	20041229	EP 2003-745893	20030403
R:			AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK	
US 2005131229	A1	20050616	US 2003-509802	20030403
CN 1646532	A	20050727	CN 2003-807596	20030403
JP 2005523911	T	20050811	JP 2003-582155	20030403
IN 2004CN02111	A	20060303	IN 2004-CN2111	20040922
PRIORITY APPLN. INFO.:			JP 2002-102456	20020404
			WO 2003-JP4259	20030403
OTHER SOURCE(S):		MARPAT 139:307792		
GI				



AB 2,6-Dihalopurines (I; X1, X2 = halogen; e.g., 2,6-dichloropurine) are prepared in high yield and selectivity by the regioselective halogenation of a 2-amino-6-halopurine (II, III; R = H, acyl; e.g., 9-acetyl-2-amino-6-chloropurine) with a halosilane (e.g., dichlorodimethylsilane) and an agent for the diazo reaction (e.g., isoamyl nitrite).

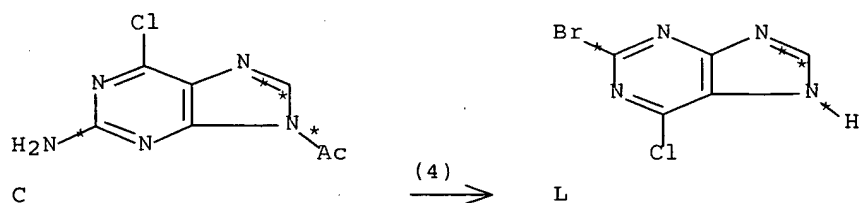
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(2) OF 6 ...C ==> E



RX(2) RCT C 470483-92-2
 RGT F 75-77-4 Me3SiCl, G 110-46-3 Isoamyl nitrite
 PRO E 5451-40-1
 CAT 56-34-8 Et4N Cl
 SOL 142-82-5 Heptane
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 60 deg C
 SUBSTAGE(3) 10 hours
 NTE optimization study

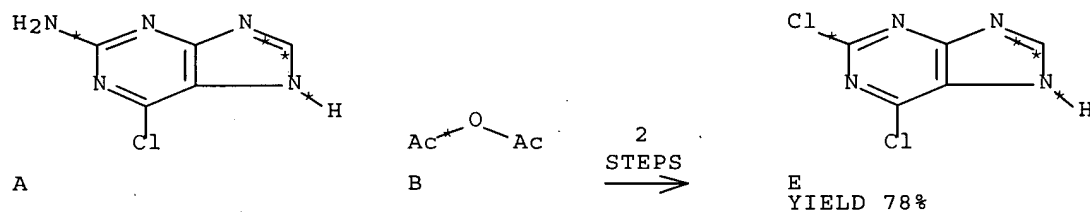
RX(4) OF 6 ...C ==> L



RX(4) RCT C 470483-92-2
 RGT M 2857-97-8 Me3SiBr, G 110-46-3 Isoamyl
 nitrite
 PRO L 500797-85-3
 SOL 109-99-9 THF
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 19 hours, 20 - 25 deg C

RX(5) OF 6 COMPOSED OF RX(1), RX(2)

RX(5) A + B ==> E

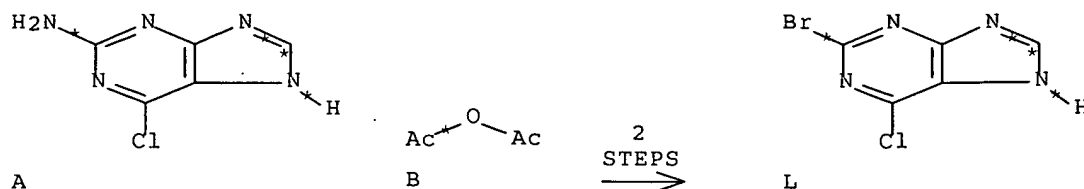


RX(1) RCT A 10310-21-1, B 108-24-7
 PRO C 470483-92-2
 SOL 127-19-5 AcNMe2
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 60 deg C
 SUBSTAGE(3) 4 hours

RX(2) RCT C 470483-92-2
 RGT F 75-77-4 Me3SiCl, G 110-46-3 Isoamyl
 nitrite
 PRO E 5451-40-1
 CAT 56-34-8 Et4N Cl
 SOL 142-82-5 Heptane
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 60 deg C
 SUBSTAGE(3) 10 hours
 NTE optimization study

RX(6) OF 6 COMPOSED OF RX(1), RX(4)

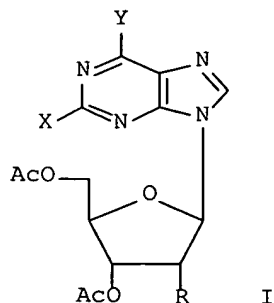
RX(6) A + B ==> L



RX(1) RCT A 10310-21-1, B 108-24-7
 PRO C 470483-92-2
 SOL 127-19-5 AcNMe₂
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 60 deg C
 SUBSTAGE(3) 4 hours

RX(4) RCT C 470483-92-2
 RGT M 2857-97-8 Me₃SiBr, G 110-46-3 Isoamyl
 nitrite
 PRO L 500797-85-3
 SOL 109-99-9 THF
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 19 hours, 20 - 25 deg C

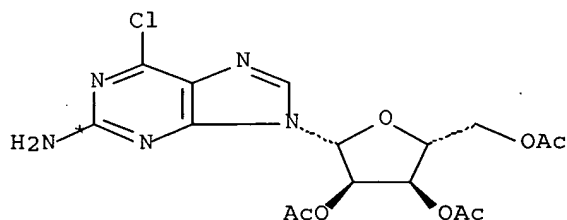
L47 ANSWER 5 OF 11 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 138:153761 CASREACT Full-text
 TITLE: Nucleic Acid Related Compounds. 118. Nonaqueous
 Diazotization of Aminopurine Derivatives. Convenient
 Access to 6-Halo- and 2,6-Dihalopurine Nucleosides and
 2'-Deoxynucleosides with Acyl or Silyl Halides
 AUTHOR(S): Francom, Paula; Robins, Morris J.
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, Brigham
 Young University, Provo, UT, 84602-5700, USA
 SOURCE: Journal of Organic Chemistry (2003), 68(2), 666-669
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



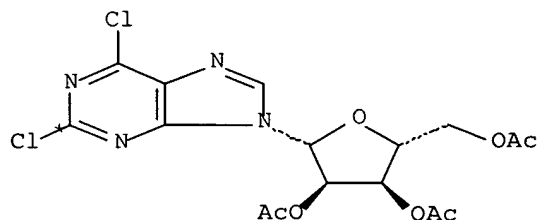
AB Treatment of 9-(2,3,5-tri-O-acetyl- β -D-ribofuranosyl)-2-amino-6-chloropurine with TMS-Cl and benzyltriethylammonium nitrite (BTEA-NO₂) in dichloromethane gave the crystalline 2,6-dichloropurine nucleoside I (R = OAc, X = Y = Cl), and acetyl chloride/BTEA-NO₂ was equally effective (.apprx.85%, without chromatog.). TMS-Br/tert-Bu nitrite/dibromomethane gave crystalline 2-bromo-6-chloro analog I (R = OAc, X = Br, Y = Cl) (85%). (Chloro or bromo)-dediazonation of 3',5'-di-O-acetyl-2'-deoxyadenosine gave chloro I (R = X = H, Y = Cl) (63%) or bromo I (R = X = H, Y = Br) (80%) purine deoxynucleosides, and 2',3',5'-tri-O-acetyladenosine was converted into the 6-chloropurine nucleoside I (R = OAc, X = H, Y = Cl) (71%).

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 9 A ==> B



A



B

YIELD 86%

RX(1) RCT A 16321-99-6

STAGE(1)

RGT C 75-77-4 Me₃SiCl, D 121699-36-3
Benzenemethanaminium, N,N,N-triethyl-, nitrite
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 1 hour, room temperature
SUBSTAGE(2) 15 minutes

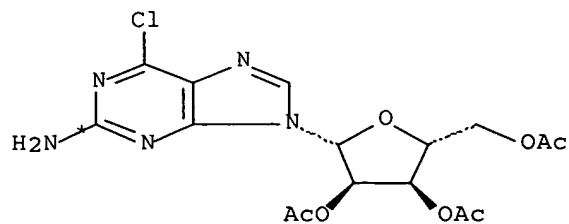
STAGE(2)

RGT E 144-55-8 NaHCO₃
SOL 7732-18-5 Water, 75-09-2 CH₂Cl₂

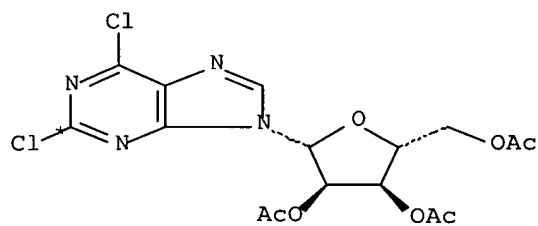
PRO B 3056-18-6

NTE yield depends on temp.

RX(2) OF 9 A ==> B



A

(2) \longrightarrow 

B

YIELD 84%

RX(2) RCT A 16321-99-6

STAGE(1)

RGT H 75-36-5 AcCl

SOL 75-09-2 CH₂Cl₂

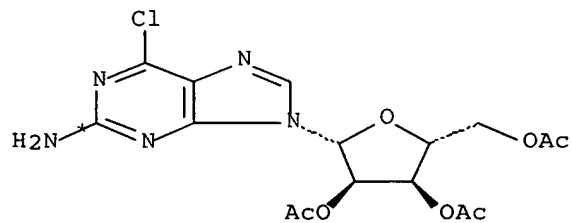
CON 15 minutes

STAGE(2)

RGT D 121699-36-3 Benzenemethanaminium,
N,N,N-triethyl-, nitriteSOL 75-09-2 CH₂Cl₂

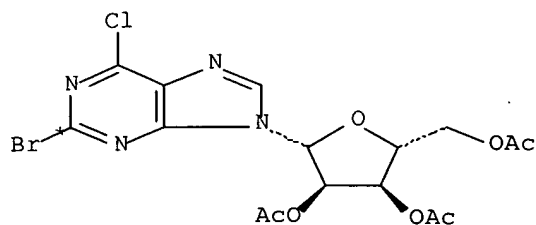
PRO B 3056-18-6

RX(3) OF 9 A ==> I



A

(3) \longrightarrow



I
YIELD 85%

RX(3) RCT A 16321-99-6

STAGE(1)

RGT J 2857-97-8 Me3SiBr, K 540-80-7 t-BuONO

SOL 74-95-3 CH2Br2

CON 1 hour, room temperature

STAGE(2)

RGT E 144-55-8 NaHCO3

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

PRO I 40896-58-0

L47 ANSWER 6 OF 11 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 138:153765 CASREACT Full-text

TITLE: Poly-amino-oligonucleotides and their combinatorial libraries

AUTHOR(S): Szmanda, Anna; Markiewicz, Maria; Godzina, Przemyslaw; Markiewicz, Wojciech T.

CORPORATE SOURCE: Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, PL-61704, Pol.

SOURCE: Collection Symposium Series (2002), 5 (Chemistry of Nucleic Acid Components), 16-26

CODEN: CSYSFN

PUBLISHER: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

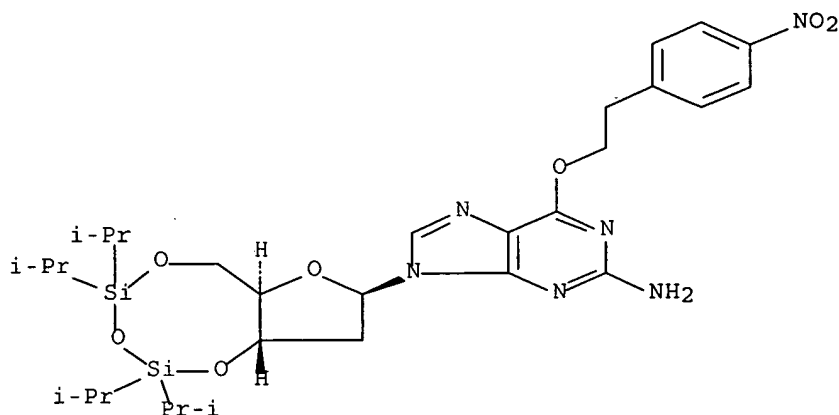
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Synthesis of oligonucleotides modified with natural polyamines at nucleobases in positions that do not interfere with Watson-Crick type base pairing was accomplished by phosphoramidite approach using appropriately protected poly-amino-nucleoside 3'-phosphoramidites. The effect of polyamine modification on DNA duplex formation was studied using a small combinatorial library for spermine modified cytosine deoxynucleoside units. All poly-amino-oligonucleotides from this library were synthesized sep., and their ability to form duplexes with a complementary non-modified oligodeoxyribonucleotide was checked by measuring their melting temps. corroborating strong stabilizing effect of polyamine modification. The obtained results indicate that combinatorial approach can be useful in studying properties of modified oligonucleotides that might be otherwise difficult to predict when one would try to apply simple stability rules drawn on the basis of study of model oligonucleotides.

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(7) OF 29 ...Q + R ==> S...



Q

STRUCTURE
DIAGRAM
IS NOT
AVAILABLE

R: CM 1

STRUCTURE
DIAGRAM
IS NOT
AVAILABLE

R: CM 3

RX(7) RCT Q 195875-07-1, R 130495-33-9

STAGE(1)

RGT T 540-80-7 t-BuONO

SOL 108-88-3 PhMe

CON 2 hours, -5 - 0 deg C

STAGE(2)

RGT U 7664-39-3 HF

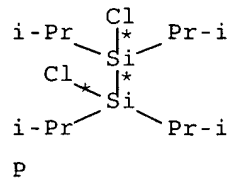
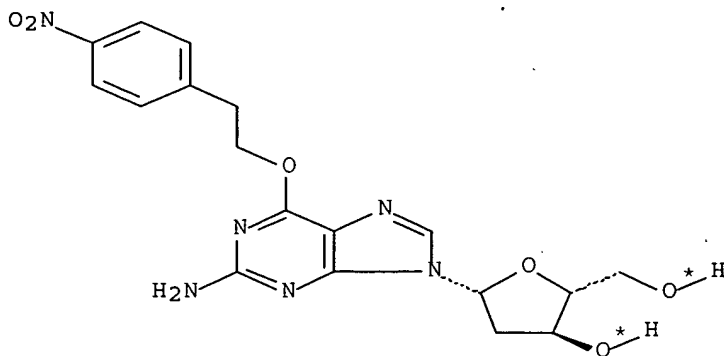
SOL 110-86-1 Pyridine

CON 160 minutes

PRO S 132183-39-2

RX(16) OF 29 COMPOSED OF RX(6), RX(7)

RX(16) O + P + R ==> S



O

STRUCTURE
DIAGRAM
IS NOT
AVAILABLE

R: CM 1

STRUCTURE
DIAGRAM
IS NOT
AVAILABLE

R: CM 3

RX(6) RCT O 86137-72-6, P 55642-25-6
PRO Q 195875-07-1
SOL 110-86-1 Pyridine
CON 2.5 hours, room temperature
NTE stereoselective

RX(7) RCT Q 195875-07-1, R 130495-33-9

STAGE(1)

RGT T 540-80-7 t-BuONO
SOL 108-88-3 PhMe
CON 2 hours, -5 - 0 deg C

STAGE(2)

RGT U 7664-39-3 HF
SOL 110-86-1 Pyridine
CON 160 minutes

PRO S 132183-39-2

RX(17) OF 29 COMPOSED OF RX(7), RX(8)
RX(17) Q + R + G ==> W

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

STRUCTURE	STRUCTURE
DIAGRAM	DIAGRAM
IS NOT	IS NOT
AVAILABLE	AVAILABLE
R: CM 1	R: CM 3

RX(7) RCT Q 195875-07-1, R 130495-33-9

STAGE(1)

RGT T 540-80-7 t-BuONO
 SOL 108-88-3 PhMe
 CON 2 hours, -5 - 0 deg C

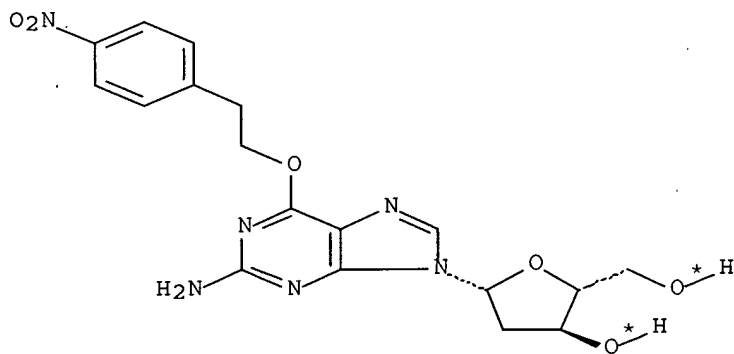
STAGE(2)

RGT U 7664-39-3 HF
 SOL 110-86-1 Pyridine
 CON 160 minutes

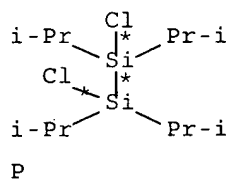
PRO S 132183-39-2

RX(8) RCT S 132183-39-2, G 40615-36-9
 PRO W 153527-28-7
 SOL 110-86-1 Pyridine
 CON 3 hours, room temperature

RX(24) OF 29 COMPOSED OF RX(6), RX(7), RX(8)
 RX(24) O + P + R + G ==> W



O



STRUCTURE	STRUCTURE
DIAGRAM	DIAGRAM
IS NOT	IS NOT
AVAILABLE	AVAILABLE
R: CM 1	R: CM 3

RX(6) RCT O 86137-72-6, P 55642-25-6
 PRO Q 195875-07-1
 SOL 110-86-1 Pyridine
 CON 2.5 hours, room temperature
 NTE stereoselective

RX(7) RCT Q 195875-07-1, R 130495-33-9

STAGE(1)

RGT T 540-80-7 t-BuONO
 SOL 108-88-3 PhMe
 CON 2 hours, -5 - 0 deg C

STAGE(2)

RGT U 7664-39-3 HF
 SOL 110-86-1 Pyridine
 CON 160 minutes

PRO S 132183-39-2

RX(8) RCT S 132183-39-2, G 40615-36-9
 PRO W 153527-28-7
 SOL 110-86-1 Pyridine
 CON 3 hours, room temperature

L47 ANSWER 7 OF 11 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 132:222784 CASREACT Full-text

TITLE: Facile conversion of 4-endo-hydroxy-2-oxabicyclo[3.3.0]oct-7-en-3-one into carbocyclic 2'-deoxyribonucleoside analogs

AUTHOR(S): Dhanda, Anupma; Knutsen, Lars J. S.; Nielsen, May-Britt; Roberts, Stanley M.; Varley, David R.

CORPORATE SOURCE: Department of Chemistry, University of Liverpool, Liverpool, L69 7ZD, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (23), 3469-3475

CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

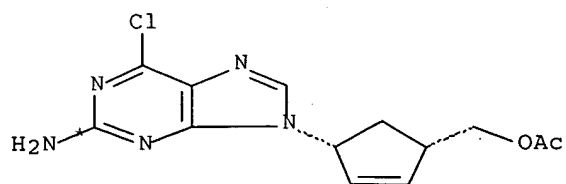
DOCUMENT TYPE: Journal

LANGUAGE: English

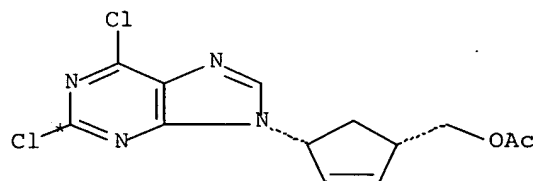
AB The readily available 3,5-syn-disubstituted cyclopentenenes react with N-bromosuccinimide (or N-bromoacetamide) and silver acetate in glacial acetic acid in a highly stereoselective manner to furnish the bromoacetates in which after hydrodebromination provided the corresponding 2'-deoxyribonucleoside analogs.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(9) OF 99 ...K ==> X...

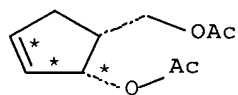


K

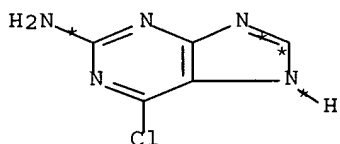
(9)
→X
YIELD 61%

RX(9) RCT K 162992-44-1
 RGT Y 75-77-4 Me3SiCl, Z 110-46-3 Isoamyl
 nitrite
 PRO X 261528-53-4
 SOL 75-09-2 CH2Cl2

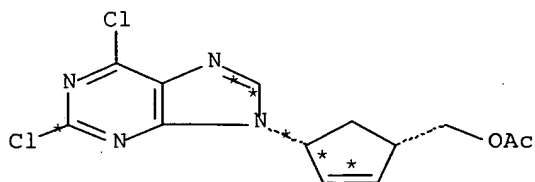
RX(26) OF 99 COMPOSED OF RX(3), RX(9)
 RX(26) I + J ==> X



I



J

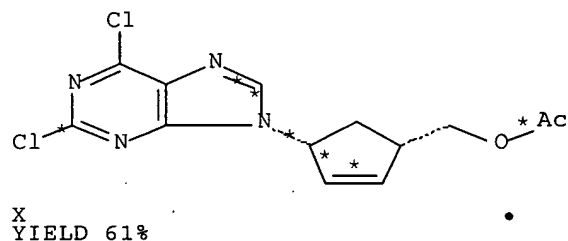
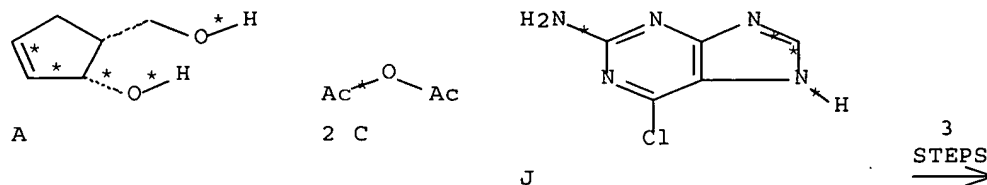
2
STEPS
→X
YIELD 61%

RX(3) RCT I 178456-34-3, J 10310-21-1
 RGT L 7646-69-7 NaH
 PRO K 162992-44-1
 CAT 14221-01-3 Pd(PPh₃)₄
 SOL 68-12-2 DMF

RX(9) RCT K 162992-44-1
 RGT Y 75-77-4 Me₃SiCl, Z 110-46-3 Isoamyl
 nitrite
 PRO X 261528-53-4
 SOL 75-09-2 CH₂Cl₂

RX(44) OF 99 COMPOSED OF RX(2), RX(3), RX(9)

RX(44) A + 2 C + J ==> X



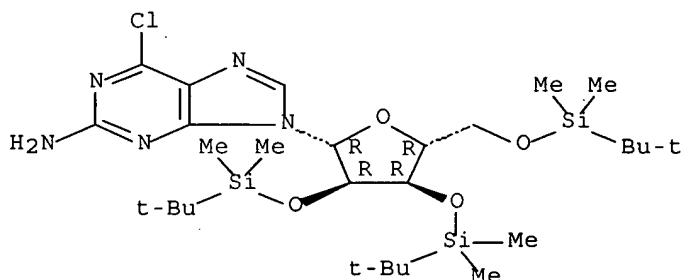
RX(2) RCT A 143395-28-2, C 108-24-7
 RGT F 1122-58-3 4-DMAP
 PRO I 178456-34-3
 SOL 110-86-1 Pyridine

RX(3) RCT I 178456-34-3, J 10310-21-1
 RGT L 7646-69-7 NaH
 PRO K 162992-44-1
 CAT 14221-01-3 Pd(PPh₃)₄
 SOL 68-12-2 DMF

RX(9) RCT K 162992-44-1
 RGT Y 75-77-4 Me₃SiCl, Z 110-46-3 Isoamyl
 nitrite
 PRO X 261528-53-4
 SOL 75-09-2 CH₂Cl₂

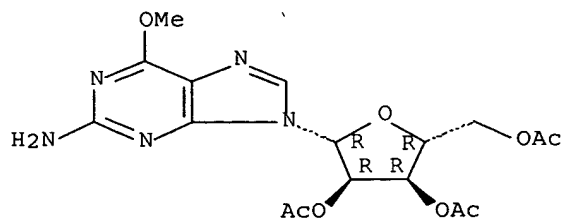
ACCESSION NUMBER: 2005:1144455 CAPLUS Full-text
 DOCUMENT NUMBER: 144:7021
 TITLE: Reaction of O6-methyl-guanosine with **nitrite**
 in the presence of carboxylic acid: synthesis of the
 purin-2-yl carboxylate
 AUTHOR(S): Maruyama, Tokumi; Moriwaka, Nobuyasu; Demizu, Yosuke;
 Ohtsuka, Masami
 CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Tokushima Bunri
 University, Sanuki City, Kagawa, 769-2193, Japan
 SOURCE: Tetrahedron Letters (2005), 46(47), 8225-8228
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 144:7021
 ED Entered STN: 26 Oct 2005
 AB O6-methyl-guanosine derivative was treated with sodium nitrite or isoamyl-
 nitrite in the presence of carboxylic acid to give the purin-2-yl carboxylate,
 an unusual product bearing a carboxylic group at the 2-position of the purine
 moiety.
 IT 141320-73-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of O6-methyl-guanosine with **nitrite** in the presence
 of carboxylic acid in synthesis of purin-2-yl carboxylates)
 RN 141320-73-2 CAPLUS
 CN 9H-Purin-2-amine, 6-chloro-9-[2,3,5-tris-O-[(1,1-
 dimethylethyl)dimethylsilyl]- β -D-ribofuranosyl]- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.



IT 92123-04-1P 869477-34-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (reaction of O6-methyl-guanosine with **nitrite** in the presence
 of carboxylic acid in synthesis of purin-2-yl carboxylates)
 RN 92123-04-1 CAPLUS
 CN Guanosine, 6-O-methyl-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

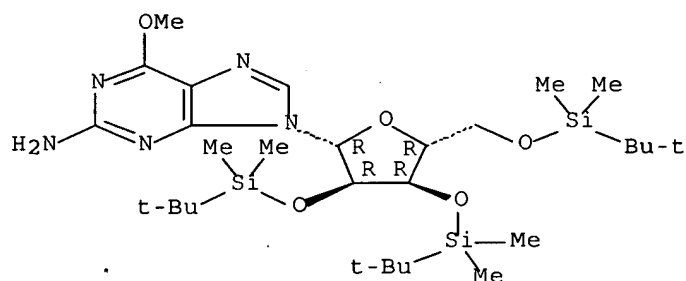
Absolute stereochemistry.



RN 869477-34-9 CAPLUS

CN Guanosine, 2',3',5'-tris-O-[(1,1-dimethylethyl)dimethylsilyl]-6-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



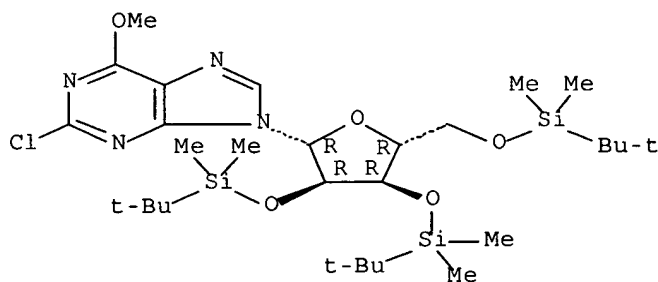
IT 869477-38-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(reaction of 06-methyl-guanosine with nitrite in the presence
of carboxylic acid in synthesis of purin-2-yl carboxylates)

RN 869477-38-3 CAPLUS

CN Inosine, 2-chloro-2',3',5'-tris-O-[(1,1-dimethylethyl)dimethylsilyl]-6-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

27

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

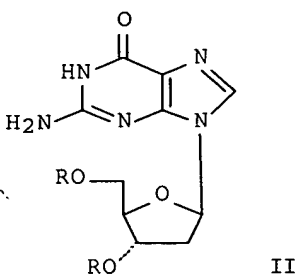
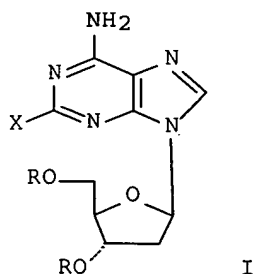
ACCESSION NUMBER: 2004:290468 CAPLUS Full-text

DOCUMENT NUMBER: 140:321651

TITLE: Process for preparing 2-halo-2'-deoxyadenosine
compounds from 2'-deoxyguanosine

INVENTOR(S): Robins, Morris J.; Janeba, Zlatko; Francom, Paula
 PATENT ASSIGNEE(S): Brigham Young University, Technology Transfer Office,
 USA
 SOURCE: PCT Int. Appl., 21 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004028462	A2	20040408	WO 2003-US30386	20030925
WO 2004028462	A3	20040610		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2540158	A1	20040408	CA 2003-2540158	20030925
AU 2003275267	A1	20040419	AU 2003-275267	20030925
EP 1556400	A2	20050727	EP 2003-759541	20030925
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006508183	T	20060309	JP 2005-501990	20030925
US 2007032645	A1	20070208	US 2006-529106	20061009
PRIORITY APPLN. INFO.:			US 2002-413915P	P 20020925
			US 2002-416329P	P 20021004
			WO 2003-US30386	W 20030925
OTHER SOURCE(S): MARPAT 140:321651				
ED Entered STN: 08 Apr 2004				
GI				



AB The present invention discloses a method for preparing 2-halo-6-aminopurines, such as I [R = H, protecting group; X = halogen] and more specifically for preparing the clin. agent cladribine I [R = H, X = Cl], a drug of choice against hairy-cell leukemia and other neoplasms, from 2-amino-6-oxopurines, such as II [R = COMe, CPh (III)]. According to the methods of the present invention, the 6-oxo group of III is converted to a 6-(substituted oxy) leaving group, or alternatively to a 6-chloro leaving group, the 2-amino group

is replaced with a 2-chloro group, the 6-(substituted oxy) leaving group, or alternatively the 6-chloro leaving group, is replaced with a 6-amino group or, alternatively, a 2,6-dichloro substituted compound is selectively replaced group, and the protecting groups are removed.

IT 24638-92-4P 69992-11-6P 119771-85-6P

500225-56-9P 500225-57-0P 500225-61-6P

500225-62-7P

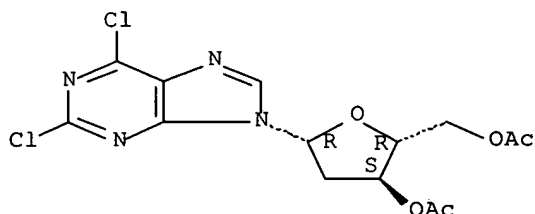
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 2-halo-2'-deoxyadenosine compds. from 2'-deoxyguanosine)

RN 24638-92-4 CAPLUS

CN 9H-Purine, 2,6-dichloro-9-(3,5-di-O-acetyl-2-deoxy- β -D-erythro-pentofuranosyl)- (9CI) (CA INDEX NAME)

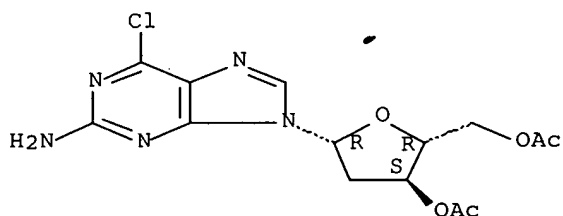
Absolute stereochemistry.



RN 69992-11-6 CAPLUS

CN 9H-Purin-2-amine, 6-chloro-9-(3,5-di-O-acetyl-2-deoxy- β -D-erythro-pentofuranosyl)- (9CI) (CA INDEX NAME)

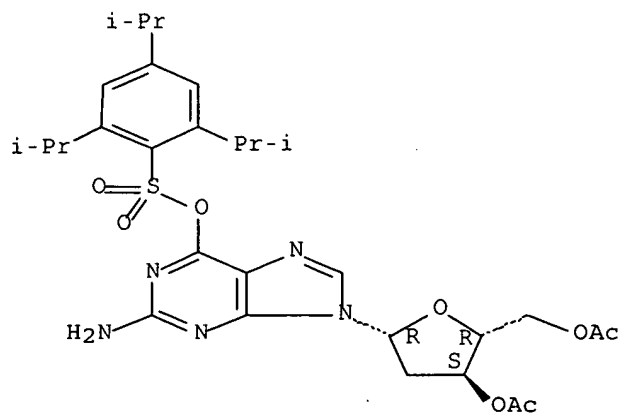
Absolute stereochemistry.



RN 119771-85-6 CAPLUS

CN Guanosine, 2'-deoxy-, 3',5'-diacetate 6-[2,4,6-tris(1-methylethyl)benzenesulfonate] (9CI) (CA INDEX NAME)

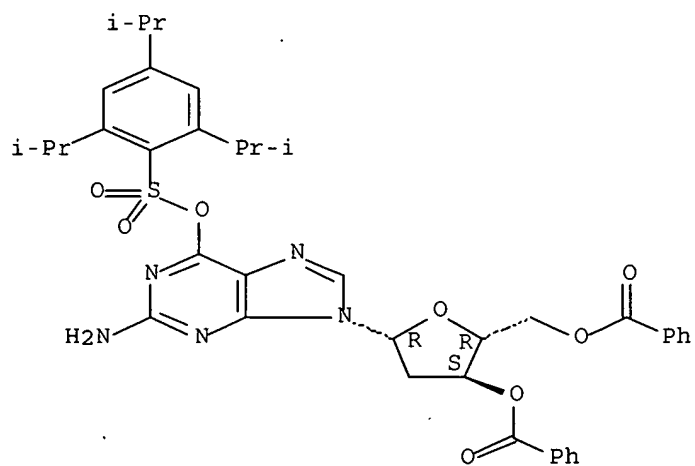
Absolute stereochemistry.



RN 500225-56-9 CAPLUS

CN Guanosine, 2'-deoxy-, 3',5'-dibenzoate 6-[2,4,6-tris(1-methylethyl)benzenesulfonate] (9CI) (CA INDEX NAME)

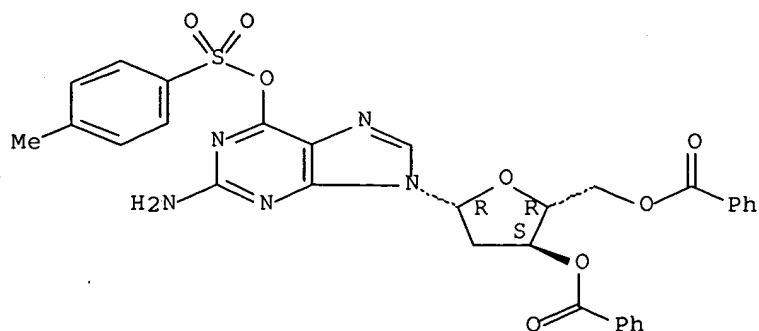
Absolute stereochemistry.



RN 500225-57-0 CAPLUS

CN Guanosine, 2'-deoxy-, 3',5'-dibenzoate 6-(4-methylbenzenesulfonate) (9CI)
(CA INDEX NAME)

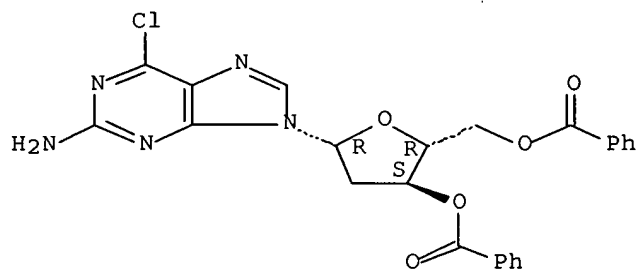
Absolute stereochemistry.



RN 500225-61-6 CAPLUS

CN 9H-Purin-2-amine, 6-chloro-9-(3,5-di-O-benzoyl-2-deoxy-beta-D-erythro-pentofuranosyl)- (9CI) (CA INDEX NAME)

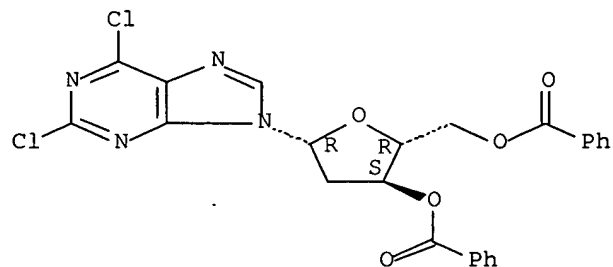
Absolute stereochemistry.



RN 500225-62-7 CAPLUS

CN 9H-Purine, 2,6-dichloro-9-(3,5-di-O-benzoyl-2-deoxy-beta-D-erythro-pentofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 3056-18-6P 4291-63-8P 40896-58-0P

500225-58-1P 500225-59-2P 500225-60-5P

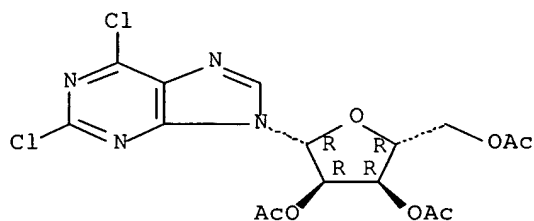
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of 2-halo-2'-deoxyadenosine compds. from 2'-deoxyguanosine)

RN 3056-18-6 CAPLUS

CN 9H-Purine, 2,6-dichloro-9-(2,3,5-tri-O-acetyl-beta-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

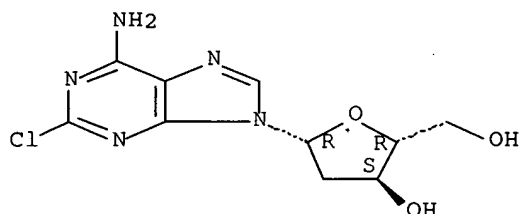
Absolute stereochemistry.



RN 4291-63-8 CAPLUS

CN Adenosine, 2-chloro-2'-deoxy- (7CI, 8CI, 9CI) (CA INDEX NAME)

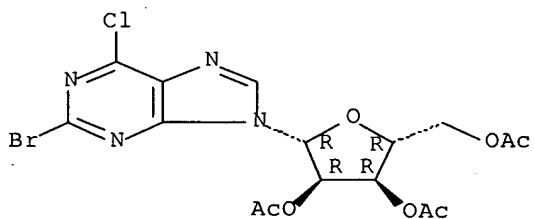
Absolute stereochemistry. Rotation (-).



RN 40896-58-0 CAPLUS

CN 9H-Purine, 2-bromo-6-chloro-9-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl) - (9CI) (CA INDEX NAME)

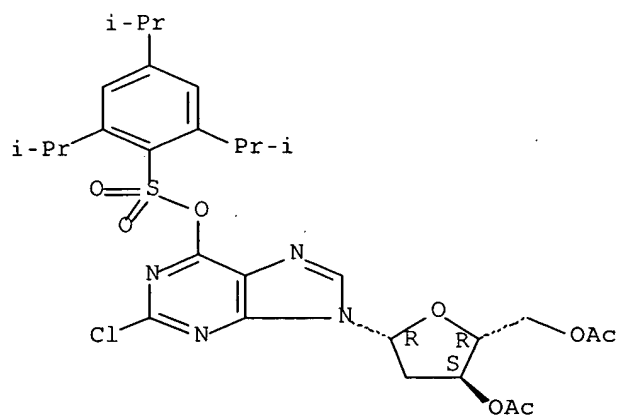
Absolute stereochemistry.



RN 500225-58-1 CAPLUS

CN Inosine, 2-chloro-2'-deoxy-, 3',5'-diacetate 6-[2,4,6-tris(1-methylethyl)benzenesulfonate] (9CI) (CA INDEX NAME)

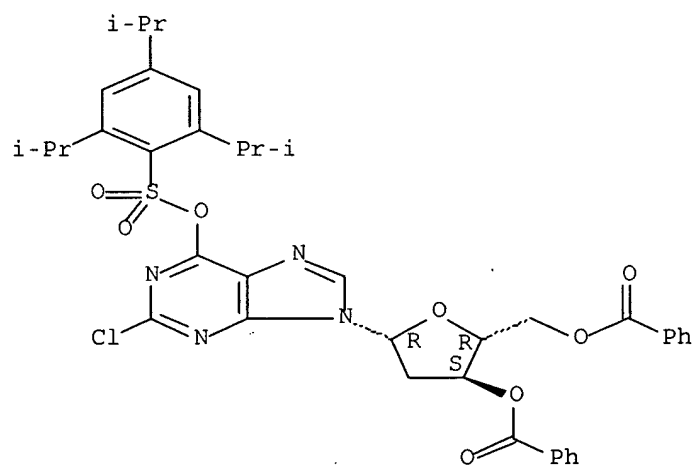
Absolute stereochemistry.



RN 500225-59-2 CAPLUS

CN Inosine, 2-chloro-2'-deoxy-, 3',5'-dibenzoate 6-[2,4,6-tris(1-methylethyl)benzenesulfonate] (9CI) (CA INDEX NAME)

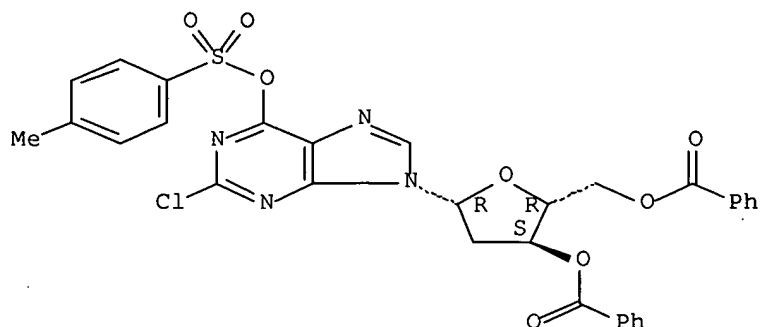
Absolute stereochemistry.



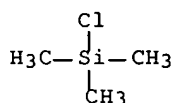
RN 500225-60-5 CAPLUS

CN Inosine, 2-chloro-2'-deoxy-, 3',5'-dibenzoate 6-(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

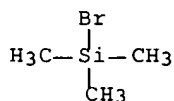
Absolute stereochemistry.



IT 75-77-4, Trimethylsilyl chloride, reactions 2857-97-8,
 Trimethylsilyl bromide 59921-49-2 69992-10-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of 2-halo-2'-deoxyadenosine compds. from 2'-deoxyguanosine)
 RN 75-77-4 CAPLUS
 CN Silane, chlorotrimethyl- (CA INDEX NAME)

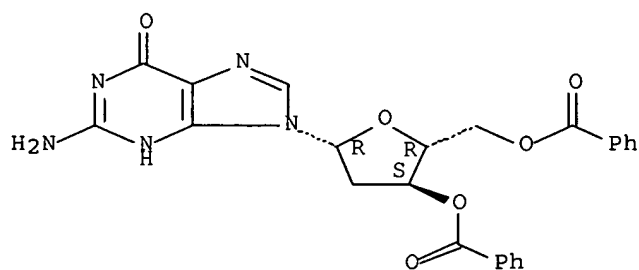


RN 2857-97-8 CAPLUS
 CN Silane, bromotrimethyl- (CA INDEX NAME)



RN 59921-49-2 CAPLUS
 CN Guanosine, 2'-deoxy-, 3',5'-dibenzoate (9CI) (CA INDEX NAME)

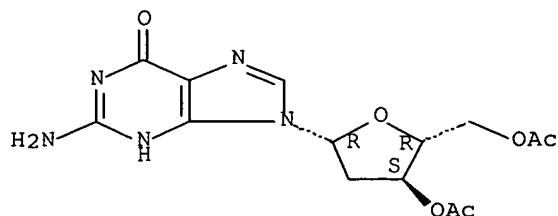
Absolute stereochemistry.



RN 69992-10-5 CAPLUS

CN Guanosine, 2'-deoxy-, 3',5'-diacetate (6CI, 7CI, 9CI) (CA INDEX NAME)

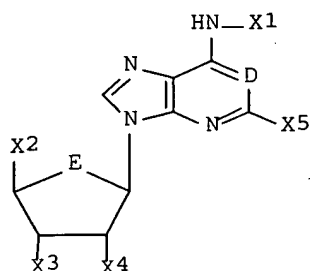
Absolute stereochemistry.



L47 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:591014 CAPLUS Full-text
 DOCUMENT NUMBER: 139:117653
 TITLE: Preparation of nucleosides as A3 adenosine receptor agonists
 INVENTOR(S): Sevillano, Luis Garcia; McGuigan, Christopher; Davies, Robin Havard
 PATENT ASSIGNEE(S): Muscagen Limited, UK
 SOURCE: PCT Int. Appl., 126 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003061670	A1	20030731	WO 2003-GB304	20030127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2474337	A1	20030731	CA 2003-2474337	20030127
EP 1469864	A1	20041027	EP 2003-700933	20030127
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006502088	T	20060119	JP 2003-561614	20030127
IN 2004KN01024	A	20060714	IN 2004-KN1024	20040720
US 2005101551	A1	20050512	US 2004-899625	20040726
PRIORITY APPLN. INFO.:			GB 2002-1849	A 20020125
			GB 2002-1919	A 20020128
			GB 2002-12438	A 20020529
			WO 2003-GB304	W 20030127

OTHER SOURCE(S): MARPAT 139:117653
 ED Entered STN: 01 Aug 2003
 GI



I

AB Adenosine analog-type A3 receptor agonists I, wherein D is N, NH; E is O, S, CH₂; X1 is heterocyclic, bicyclic; X2 is hydroxymethyl, alkoxyethyl, cycloalkoxy Me, carboxy, alkoxyethyl, cycloalkoxyethyl, aminoiminomethyl, alkylaminoiminomethyl, cycloalkylaminoiminomethyl, carbamoyl, alkylaminocarbonyl, cycloalkylaminocarbonyl, cycloalkylaminocarbonyl; X3 and X4 are each independently hydrogen, alkyl, hydroxyalkyl, alkoxyalkyl, ORa or NRaRb, where Ra and Rb are independently hydrogen, alkyl, aralkyl, carbamoyl, alkyl carbamoyl, dialkylcarbamoyl, acyl, alkoxyethyl, aralkoxyethyl, aryloxyethyl; X5 is H, halogen, alkyl, fluorinated alkyl, alkoxyalkyl, alkoxy, alkyl-ether, thioalkoxy, alkylthio, amino, alkylamino, were prepared as A3 adenosine receptor agonists. Thus, N5-(4-methyl-2-picolyl)-adenosine-5'-N-methyluronamide was prepared and tested on as A3 adenosine receptor agonist of guinea-pig trachea (IC₅₀ = 2.2 nM).

IT 565237-15-2P

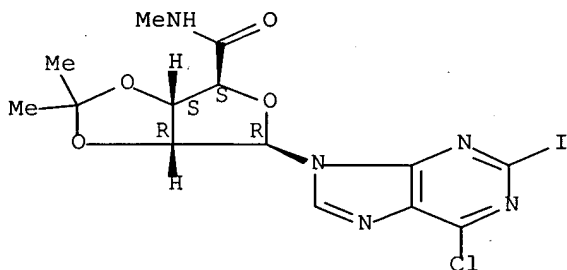
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nucleosides as a adenosine receptor agonists)

RN 565237-15-2 CAPLUS

CN β -D-Ribofuranuronamide, 1-(6-chloro-2-iodo-9H-purin-9-yl)-1-deoxy-N-methyl-2,3-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 219755-20-1

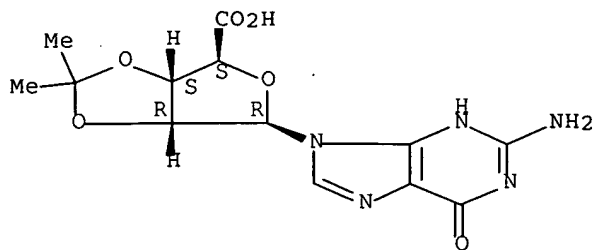
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of nucleosides as a adenosine receptor agonists)

RN 219755-20-1 CAPLUS

CN β -D-Ribofuranuronic acid, 1-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-1-deoxy-2,3-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

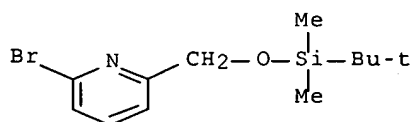


IT 150058-63-2P 565237-08-3P 565237-16-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nucleosides as a adenosine receptor agonists)

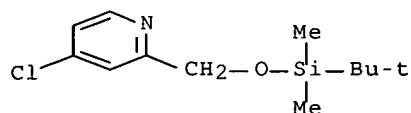
RN 150058-63-2 CAPLUS

CN Pyridine, 2-bromo-6-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl] - (CA INDEX NAME)



RN 565237-08-3 CAPLUS

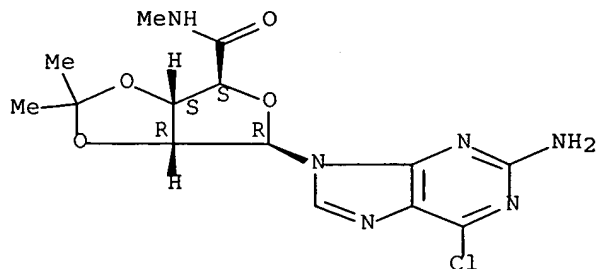
CN Pyridine, 4-chloro-2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl] - (9CI) (CA INDEX NAME)



RN 565237-16-3 CAPLUS

CN β -D-Ribofuranuronamide, 1-(2-amino-6-chloro-9H-purin-9-yl)-1-deoxy-N-methyl-2,3-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:532671 CAPLUS Full-text

DOCUMENT NUMBER: 113:132671

TITLE: Acyclic nucleotide analogs. VIII. Synthesis of N-(2-(2-phosphonylethoxy)ethyl) derivatives of heterocyclic bases

AUTHOR(S): Holy, Antonin; Rosenberg, Ivan; Dvorakova, Hana
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, 166 10, Czech.

SOURCE: Collection of Czechoslovak Chemical Communications (1990), 55(3), 809-18
CODEN: CCCCAK; ISSN: 0010-0765

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 13 Oct 1990

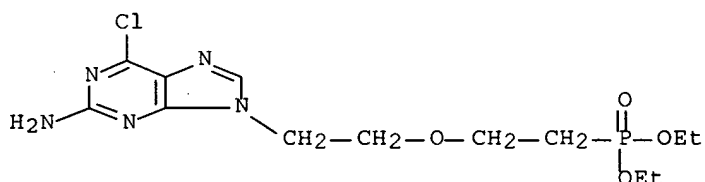
AB Reaction of bis(2-chloroethyl) ether with (EtO)₃P afforded di-Et 2-chloroethoxyethylphosphonate. This compound reacts with Na salts of heterocyclic bases to give di-Et esters of N-[2-(2-phosphonylethoxy)ethyl] derivs. of purine and pyrimidine bases. These compds. on reaction with Me₃SiBr and subsequent hydrolysis were converted into N-[2-(phosphonylethoxy)ethyl] derivs., BCH₂CH₂OCH₂CH₂P(O)(OH)₂ (B = purine or pyrimidine base).

IT 129432-02-6P 129432-03-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

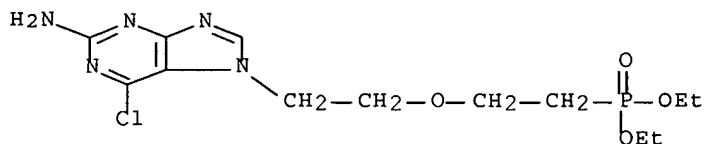
RN 129432-02-6 CAPLUS

CN Phosphonic acid, [2-[2-(2-amino-6-chloro-9H-purin-9-yl)ethoxy]ethyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 129432-03-7 CAPLUS

CN Phosphonic acid, [2-[2-(2-amino-6-chloro-7H-purin-7-yl)ethoxy]ethyl]-, diethyl ester (9CI) (CA INDEX NAME)



IT 129432-01-5P

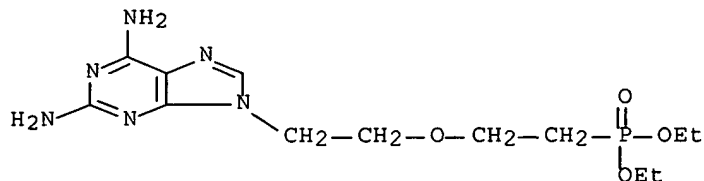
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT (Reactant or reagent)

(preparation and silylation and hydrolysis of)

RN 129432-01-5 CAPLUS

CN Phosphonic acid, [2-[2-(2,6-diamino-9H-purin-9-yl)ethoxy]ethyl]-, diethyl ester (9CI) (CA INDEX NAME)



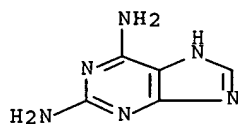
IT 1904-98-9, 1H-Purine-2,6-diamine

RL: RCT (Reactant); **RACT (Reactant or reagent)**

(reaction of, with di-Et (chloroethoxy)ethylphosphonate)

RN 1904-98-9 CAPLUS

CN 1H-Purine-2,6-diamine (9CI) (CA INDEX NAME)



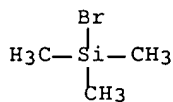
IT 2857-97-8, Bromotrimethylsilane

RL: RCT (Reactant); **RACT (Reactant or reagent)**

(reaction of, with di-Et phosphonylethoxyethyl derivs. of purine and pyrimidine bases)

RN 2857-97-8 CAPLUS

CN Silane, bromotrimethyl- (CA INDEX NAME)

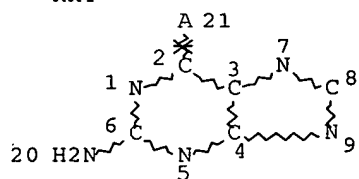


FILE 'HOME' ENTERED AT 16:52:21 ON 12 MAR 2007

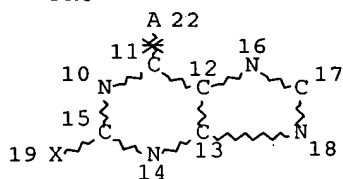
SEARCH HISTORY

=> d stat que l46; d stat que l44; d his nofile
L1 STR

RRT



PRO



NODE ATTRIBUTES:

NSPEC IS RC AT 21
NSPEC IS RC AT 22
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

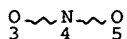
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

****MAPPINGS****

NOD SYM	ROL	NOD SYM	ROL
21 A	RRT	22 A	PRO
22 A	PRO	21 A	RRT

L4 81 SEA FILE=CASREACT SSS FUL L1 (264 REACTIONS)
L20 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

L23 76 SEA FILE=CASREACT SUB=L4 SSS FUL L20 (250 REACTIONS)
L25 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

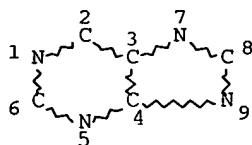
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 2

STEREO ATTRIBUTES: NONE

L28 8 SEA FILE=CASREACT SUB=L4 SSS FUL L25 (18 REACTIONS)
 L29 7 SEA FILE=CASREACT ABB=ON L28 AND L23
 L46 7 SEA FILE=CASREACT ABB=ON L29 OR (L29 AND (L23 OR L28))

L5 184754 SEA FILE=REGISTRY ABB=ON X/ELS AND SI/ELS
 L30 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

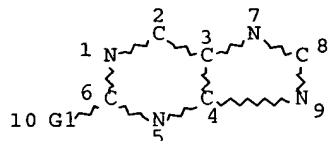
GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L31 258797 SEA FILE=REGISTRY SSS FUL L30
 L32 STR



VAR G1=NH2/X

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L35 62619 SEA FILE=REGISTRY SUB=L31 SSS FUL L32
 L36 13779 SEA FILE=REGISTRY ABB=ON L35 AND X/ELS
 L37 48840 SEA FILE=REGISTRY ABB=ON L35 NOT L36
 L38 93825 SEA FILE=CAPLUS ABB=ON L37
 L39 3461 SEA FILE=CAPLUS ABB=ON L36/P
 L40 9922 SEA FILE=CAPLUS ABB=ON L38 (L) RACT/RL
 L41 177552 SEA FILE=CAPLUS ABB=ON L5
 L42 207 SEA FILE=CAPLUS ABB=ON L39 AND L40 AND L41
 L43 56042 SEA FILE=CAPLUS ABB=ON NITRITE#/OBI
 L44 4 SEA FILE=CAPLUS ABB=ON L43 AND L42

(FILE 'HOME' ENTERED AT 15:38:00 ON 12 MAR 2007)

FILE 'CASREACT' ENTERED AT 15:38:18 ON 12 MAR 2007

L1 STR
 L2 1 SEA SSS SAM L1 (4 REACTIONS)
 D SCAN
 L3 181 SEA SSS FUL L1 (969 REACTIONS) EXTEND
 L4 81 SEA SSS FUL L1 (264 REACTIONS)
 SAVE TEMP L4 BER802FULL/A

FILE 'REGISTRY' ENTERED AT 15:42:30 ON 12 MAR 2007

L5 184754 SEA ABB=ON X/ELS AND SI/ELS
 L6 53876 SEA ABB=ON L5 AND CASREACT/LC
 SET NOTICE 50

FILE 'CASREACT' ENTERED AT 15:43:17 ON 12 MAR 2007

L7 50154 SEA ABB=ON L6
 L8 24 SEA ABB=ON L7 AND L4
 L9 2409 SEA ABB=ON L6/CAT
 L10 1 SEA ABB=ON L4 AND L9
 D SCAN
 L11 STR

FILE 'LREGISTRY' ENTERED AT 15:47:41 ON 12 MAR 2007

L12 STR
 L13 14 SEA SSS SAM L12

FILE 'CASREACT' ENTERED AT 15:48:24 ON 12 MAR 2007

L14 0 SEA SUB=L4 SSS SAM L11 (0 REACTIONS)
 L15 STR L11

FILE 'LREGISTRY' ENTERED AT 15:48:59 ON 12 MAR 2007

L16 6 SEA ABB=ON NITRATE ESTER
 D SCAN

FILE 'CASREACT' ENTERED AT 15:49:30 ON 12 MAR 2007

D L15
 L17 1 SEA SUB=L4 SSS SAM L15 (4 REACTIONS)
 D SCAN
 D SCAN L10
 D QUE L17
 E US2005-509802/APPS

FILE 'CAPLUS' ENTERED AT 16:35:37 ON 12 MAR 2007

E US2005-509802/APPS

FILE 'CASREACT' ENTERED AT 16:36:35 ON 12 MAR 2007

D QUE L11
 L18 1 SEA ABB=ON L4(L)L9
 D HIT
 D QUE L11
 SET NOTICE 20
 L19 0 SEA SUB=L4 SSS SAM L11 (0 REACTIONS)
 L20 STR L11
 L21 1 SEA SUB=L4 SSS SAM L20 (4 REACTIONS)
 D SCAN
 L22 76 SEA SUB=L4 SSS FUL L20 (250 REACTIONS) EXTEND

L23 76 SEA SUB=L4 SSS FUL L20 (250 REACTIONS)
 SAVE TEMP L23 BER802SUB1/A
 L24 21 SEA ABB=ON L23 AND L7
 L25 STR
 L26 0 SEA SUB=L4 SSS SAM L25 (0 REACTIONS)
 L27 8 SEA SUB=L4 SSS FUL L25 (18 REACTIONS) EXTEND
 L28 8 SEA SUB=L4 SSS FUL L25 (18 REACTIONS)
 SAVE TEMP L27 BER802SUB2/A
 L29 7 SEA ABB=ON L28 AND L23
 SAVE TEMP L29 BER802SUB3/A
 D SCAN

FILE 'REGISTRY' ENTERED AT 16:42:48 ON 12 MAR 2007

D SAVED
 D COST
 ACT BER645FULL/A

L30 STR
 L31 258797 SEA SSS FUL L30

 L32 STR L30
 L33 50 SEA SUB=L31 SSS SAM L32
 L34 110734 SEA SUB=L31 SSS FUL L32 EXTEND
 L35 62619 SEA SUB=L31 SSS FUL L32
 L36 13779 SEA ABB=ON L35 AND X/ELS
 L37 48840 SEA ABB=ON L35 NOT L36

FILE 'CAPLUS' ENTERED AT 16:46:11 ON 12 MAR 2007

L38 93825 SEA ABB=ON L37
 L39 3461 SEA ABB=ON L36/P
 L40 9922 SEA ABB=ON L38(L) RACT/RL
 L41 177552 SEA ABB=ON L5
 L42 207 SEA ABB=ON L39 AND L40 AND L41
 L43 56042 SEA ABB=ON NITRITE#/OBI
 L44 4 SEA ABB=ON L43 AND L42

FILE 'CASREACT' ENTERED AT 16:49:04 ON 12 MAR 2007

D STAT QUE L29

FILE 'CAPLUS' ENTERED AT 16:49:13 ON 12 MAR 2007

D STAT QUE L44

FILE 'CASREACT, CAPLUS' ENTERED AT 16:49:21 ON 12 MAR 2007

L45 11 DUP REM L29 L44 (0 DUPLICATES REMOVED)
 ANSWERS '1-7' FROM FILE CASREACT
 ANSWERS '8-11' FROM FILE CAPLUS
 D IBIB ABS HIT

FILE 'CASREACT' ENTERED AT 16:51:09 ON 12 MAR 2007

L46 7 SEA ABB=ON L29 OR (L29 AND (L23 OR L28))

FILE 'CASREACT' ENTERED AT 16:51:26 ON 12 MAR 2007

D STAT QUE L46

FILE 'CAPLUS' ENTERED AT 16:51:31 ON 12 MAR 2007

D STAT QUE L44

FILE 'CASREACT, CAPLUS' ENTERED AT 16:51:39 ON 12 MAR 2007

L47 11 DUP REM L46 L44 (0 DUPLICATES REMOVED)
 ANSWERS '1-7' FROM FILE CASREACT

ANSWERS '8-11' FROM FILE CAPLUS
D IBIB ABS HIT
D IBIB ABS HIT 2-7
D IBIB ED ABS HITSTR 8-11

FILE 'HOME' ENTERED AT 16:52:21 ON 12 MAR 2007

D STAT QUE L46

D STAT QUE L44

=>